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NEWS	3	FEB	02	Simultaneous left and right truncation (SLART) added for CERAB, COMPUAB, ELCOM, and SOLIDSTATE
NEWS	4	FEB	02	GENBANK enhanced with SET PLURALS and SET SPELLING
NEWS	5	FEB	06	Patent sequence location (PSL) data added to USGENE
NEWS	6	FEB	10	COMPENDEX reloaded and enhanced
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NEWS	20	MAR	3.0	IMSPATENTS reloaded and enhanced
NEWS		APR		CAS coverage of exemplified prophetic substances enhanced
NEWS	22	APR	0.7	STN is raising the limits on saved answers
NEWS		APR		CA/CAplus now has more comprehensive patent assignee
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NEWS		APR		USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
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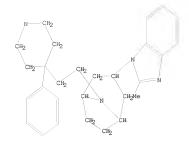
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18 19 20
ring nodes:
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 21 22 23 24 25 26 27 28 29 30 31 32
Chain bonds:
5-17 8-19 16-18 19-20 20-26 26-30
ring bonds:
1-2 1-7 2-3 3-4 3-8 4-5 5-6 6-7 7-8 9-10 9-14 9-15 10-11 10-17 11-12 12-13 13-14 15-16 16-17 21-22 21-26 22-23 23-24 24-25 25-26 27-28 27-32 28-29 29-30 30-31 31-32
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Match level: 1:1Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:CLASS 19:CLASS 20:CLASS 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 20:Atom 27:Atom 28:Atom 28:Ato

## L1 STRUCTURE UPLOADED

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chain nodes :



Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss full FULL SEARCH INITIATED 18:01:26 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 1294 TO ITERATE

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L2 1233 SEA SSS FUL L1

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 COST IN U.S. DOLLARS
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FILE COVERS 1907 - 19 May 2009 VOL 150 ISS 21 FILE LAST UPDATED: 18 May 2009 (20090518/ED) REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009 USPIO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

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reclassification data for the third quarter of 2008.

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=> d 13 abs ibib

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

AB We describe robust chemical approaches toward putative CCR5 scaffolds designed in our labs. Evaluation of analogs in the 125I-[MIP-18] binding and Ba-L-HOS antiviral assays resulted in the discovery of 64 and 68 in the 4,4-disubstituted piperidine class H, both potent CCR5 ligands (pIC50 = 8.30 and 9.00, resp.) and HIV-1 inhibitors (pIC50 = 7.80 and 7.84, resp., in Ba-L-HOS assay). In addition, 64 and 68 were bioavailable in rodents, establishing them as lead mols. for further optimization toward CCR5 clin. candidates.

2008:1154437 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 149:486141

TITLE: Discovery of Bioavailable 4,4-Disubstituted

Piperidines as Potent Ligands of the Chemokine

Receptor 5 and Inhibitors of the Human

Immunodeficiency Virus-1

AUTHOR(S): Kazmierski, Wieslaw M.; Aquino, Christopher; Chauder,

Brian A.; Deanda, Felix; Ferris, Robert;

Jones-Hertzog, Deborah K.; Kenakin, Terrence; Koble, Cecilia S.; Watson, Christian; Wheelan, Pat; Yang,

Hanbiao; Youngman, Michael

Infectious Diseases Center for Excellence in Drug CORPORATE SOURCE:

Discovery, Molecular Discovery Research, Computational and Structural Chemistry, Drug Discovery, IT ID DMPK, Metabolic Pathways Center for Excellence in Drug Discovery, GlaxoSmithKline, Research Triangle Park,

NC, 27709, USA Journal of Medicinal Chemistry (2008), 51(20),

6538-6546

CODEN: JMCMAR; ISSN: 0022-2623 PUBLISHER:

American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS

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L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2009 ACS on STN

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Compds. I [R1 = (optionally substituted) alkyl, aryl, heteroaryl, AB carbocyclyl; R2 = H, (optionally substituted) alkyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, aralkyl, heteroarylalkyl,

heteroarylcycloalkyl, aralkylcarbonyl, heteroarylsulfinyl; R3 = H, halo, cyano, trifluoromethyl, (optionally substituted) amino, acylamino, alkyl; X = C1-5 alkylene, optionally substituted with oxo or thioxo groups or halogen atoms, and optionally containing 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms; Y = carbonyl, thiocarbonyl, 1,2-dioxoethylene, oxyalkylcarbonyl, sulfinyl, sulfonyl, oxycyanoimino, (optionally substituted) aminocarbonyl, carbonylamino, aminothiocarbonyl, oxyiminomethyl, thioiminomethyl, amino(cyanoimino)methyl, (cvanoimino)methyl, amino(acvlimino)methyl, amino(sulfonylimino)methyl, amino(sulfinvlimino)methyl, amino(alkoxvimino)methyl, amino(imino)methyl, (cyanoimino) methoxy, iminomethoxy, (cyanoimino) methanethivl, alkylcarbonyloxy; A = saturated, partially saturated, or aromatic monocyclic with 5-6 atoms or a bicyclic ring with 8-10 members containing 0-5 nitrogen, oxygen, and/or sulfur atoms] such as II are prepared I are prepared as Ccr5 antagonists for the treatment of viral infections, (particularly HIV infection), related syndromes such as AIDS-related complex (ARC), progressive generalized lymphadenopathy, Kaposi's sarcoma, and neurol. conditions, and other diseases such as multiple sclerosis, rheumatoid arthritis, Crohn's disease, and immune-mediated disorders. The invention compds. have pIC50 values of ≥5 in assays for Ccr5 antagonism. Piperidineacetaldehyde III is prepared in four steps from 4-phenyl-4-piperidinecarbonitrile by protection of the piperidine with Boc anhydride, reduction of the nitrile with dissobutylaluminum hydride, Wittig olefination with methoxymethylphosphonium chloride, and hydrolysis of the enol ether with catalytic p-toluenesulfonic acid monohydrate. The hydrochloride of endo-(benzimidazolyl)azabicyclooctane IV is prepared in five steps from tert-Bu endo-3-oxo-8-azabicyclo[3.2.1]octane-8-carboxylate; reductive amination with benzylamine, reductive cleavage of the benzyl group by palladium-mediated hydrogenation, a nucleophilic aryl substitution reaction with 1-fluoro-2-nitrobenzene, reduction of the nitro group by hydrogenation over palladium on carbon, and treatment with tri-Et orthoacetate followed by treatment with hydrochloric acid in ethanol. Coupling of III and IV by reductive amination with sodium triacetoxyborohydride, cleavage of the Boc group with hydrochloric acid in dioxane, and acylation with pivaloyl chloride and triethylamine yields II. ACCESSION NUMBER: 2004:534173 CAPLUS DOCUMENT NUMBER: 141:89016 TITLE: Preparation of benzimidazolylazabicyclooctylethylpiperidines as Ccr5 antagonists for the treatment of HIV infection INVENTOR(S): Kazmierski, Wieslaw Mieczyslaw; Aquino, Christopher Joseph: Bifulco, Neil: Boros, Eric Eugene: Chauder, Brian Andrew; Chong, Pek Yoke; Duan, Maosheng; Deanda, Felix, Jr.; Koble, Cecilia Suarez; Mclean, Ed Williams; Peckham, Jennifer Poole; Perkins, Angilique C.; Thompson, James Benjamin; Vanderwall, Dana PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA; et al.; et al. SOURCE: PCT Int. Appl., 859 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: KIND DATE APPLICATION NO. DATE PATENT NO.

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WO	2004054974				A2		2004	0701	WO 2003-US39644						20031212		
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